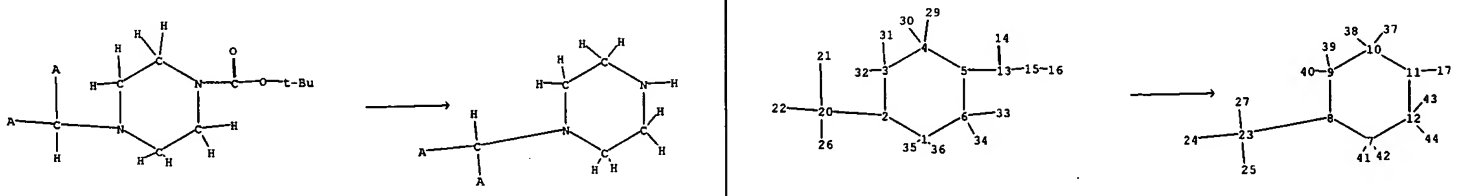
C:\Program Files\Stnexp\Queries\10076448.str

CAS React NP



chain nodes :
13 14 15 16 17 20 23 26 27 29 30 31 32 33 34 35 36 37 38 39 40 41
42 43 44
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12
ring/chain nodes :
21 22 24 25
chain bonds :
1-35 1-36 2-20 3-31 3-32 4-29 4-30 5-13 6-33 6-34 7-41 7-42 8-23 9-39 9-40
10-37 10-38 11-17 12-43 12-44 13-14 13-15 15-16 20-21 20-22 20-26 23-24 23-25
23-27
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
1-2 1-6 2-3 2-20 3-4 4-5 5-6 5-13 7-8 7-12 8-9 8-23 9-10 10-11 11-12 13-14
13-15 20-21 20-22 23-24 23-25
exact bonds :
1-35 1-36 3-31 3-32 4-29 4-30 6-33 6-34 7-41 7-42 9-39 9-40 10-37 10-38
11-17 12-43 12-44 15-16 20-26 23-27

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 20:CLASS 21:CLASS 22:CLASS
23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS
33:CLASS 34:CLASS 35:CLASS 36:CLASS 37:CLASS 38:CLASS 39:CLASS 40:CLASS 41:CLASS
42:CLASS 43:CLASS 44:CLASS
fragments assigned product role:
containing 7
fragments assigned reactant/reagent role:
containing 1

```
=>
Uploading 10076448.str

L3      STRUCTURE UPLOADED

=> s l3
SAMPLE SEARCH INITIATED 18:16:31 FILE 'CASREACT'
SCREENING COMPLETE -     93 REACTIONS TO VERIFY FROM     10 DOCUMENTS

100.0% DONE     93 VERIFIED       0 HIT RXNS                    0 DOCS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED VERIFICATIONS:      1282 TO     2438
PROJECTED ANSWERS:               0 TO        0

L4            0 SEA SSS SAM L3 (     0 REACTIONS)

=> s l3 sss full
FULL SEARCH INITIATED 18:16:39 FILE 'CASREACT'
SCREENING COMPLETE -   2203 REACTIONS TO VERIFY FROM    180 DOCUMENTS

100.0% DONE   2203 VERIFIED      26 HIT RXNS                    2 DOCS
SEARCH TIME: 00.00.01

L5            2 SEA SSS FUL L3 (    26 REACTIONS)

=> d 1-2 crd
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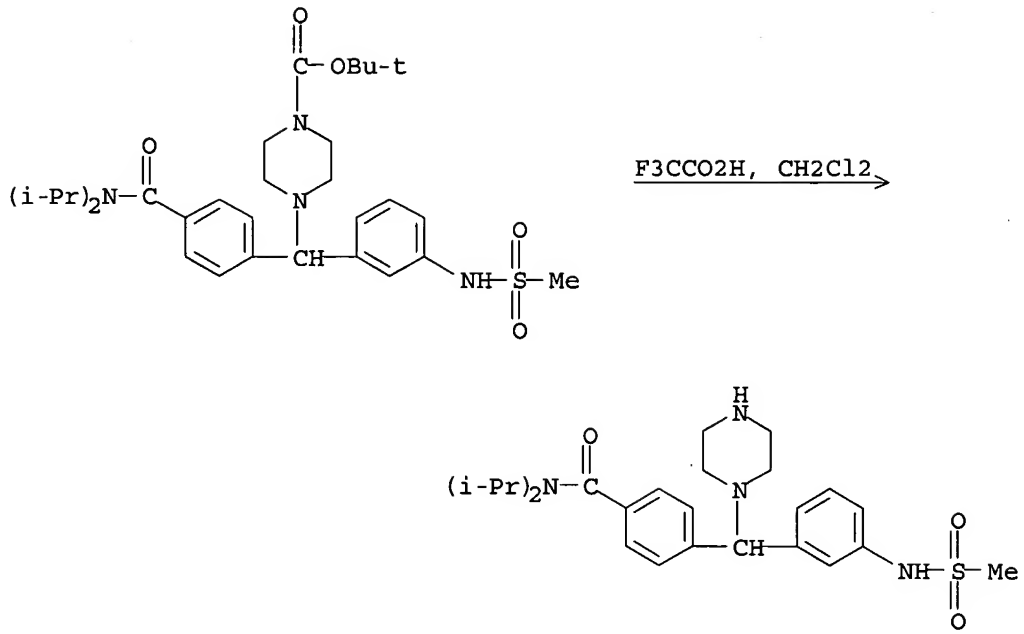
L5 ANSWER 1 OF 2 CASREACT COPYRIGHT 2003 ACS

RX(18) OF 48



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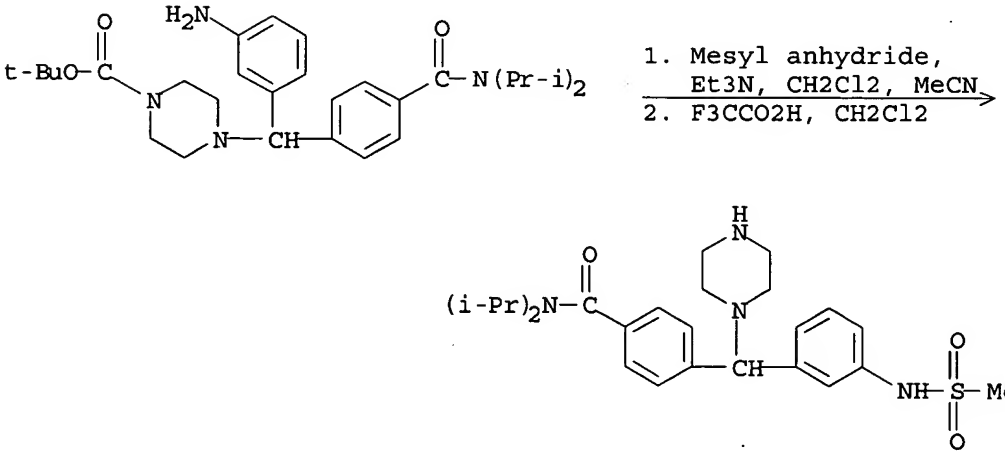
RX(37) OF 48 - 2 STEPS



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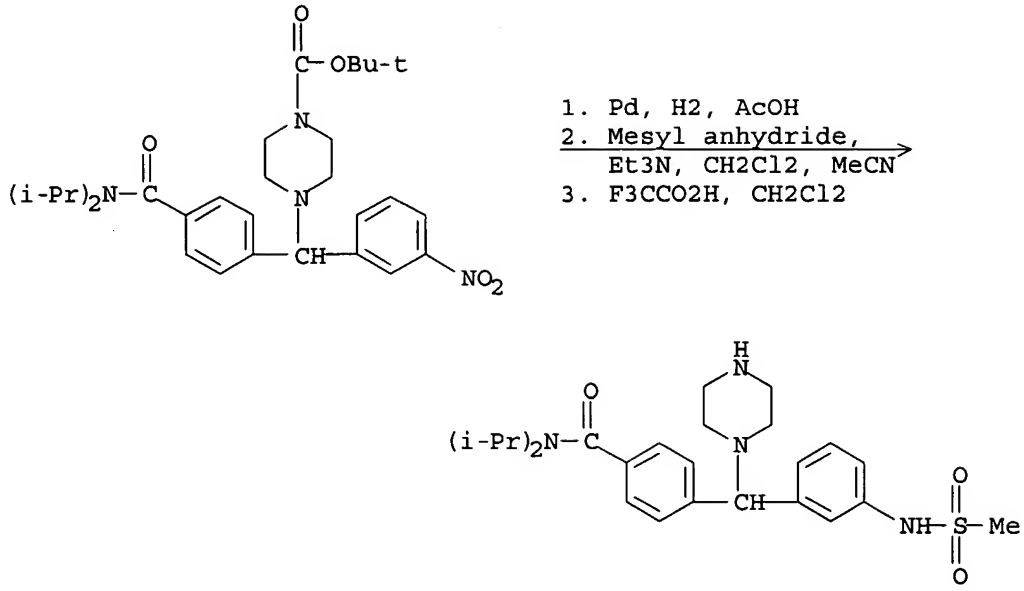
RX(44) OF 48 - 3 STEPS



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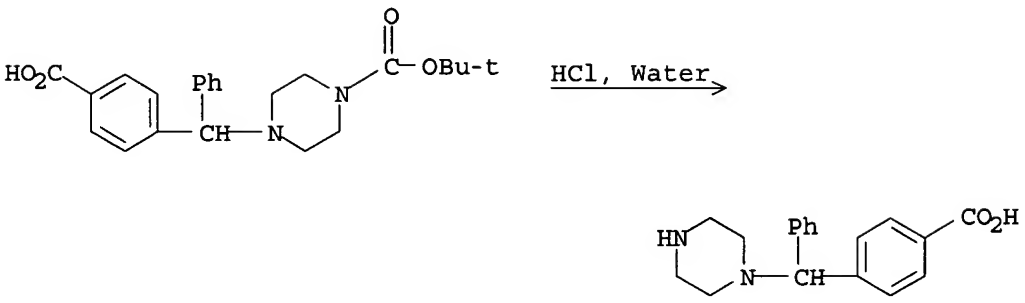
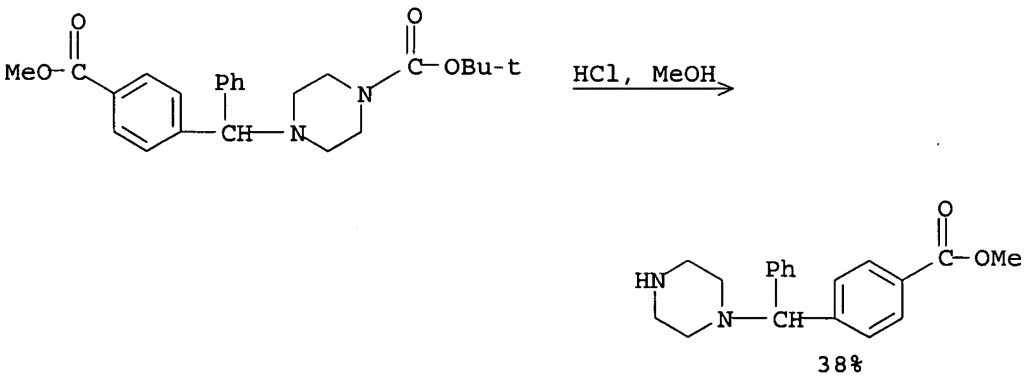
L5 ANSWER 2 OF 2 CASREACT COPYRIGHT 2003 ACS

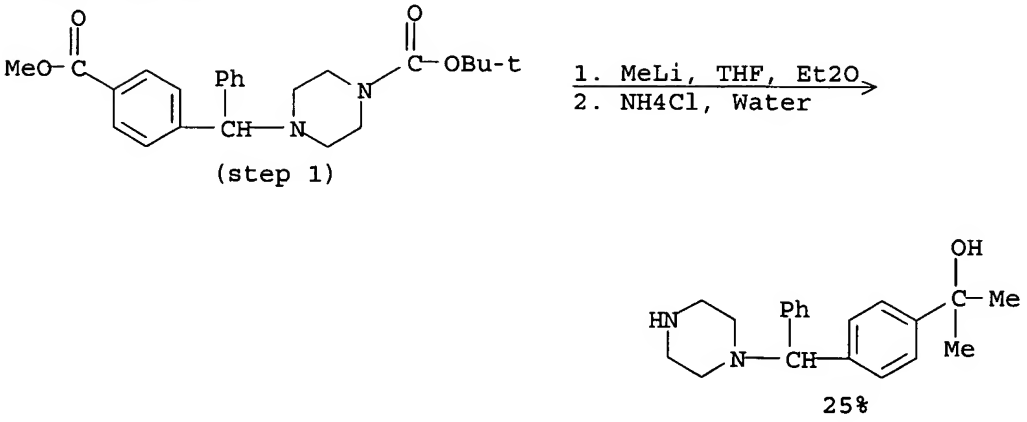
RX(19) OF 401



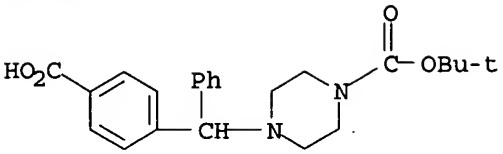
RX(22) OF 401



RX(23) OF 401

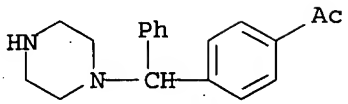


RX(24) OF 401



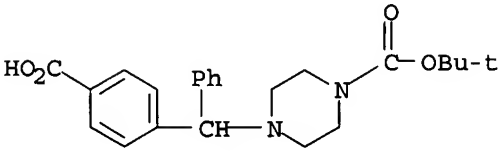
(step 1)

1. MeLi, THF, Et2O
2. Me3SiCl
3. NH4Cl, Water



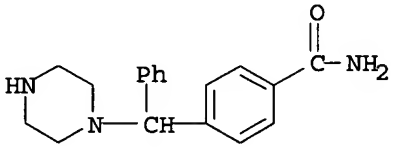
76%

RX(25) OF 401



(step 1)

1. Et3N, ClCO2Bu-i, THF
2. NH3, CH2Cl2
3. F3CCO2H, CH2Cl2



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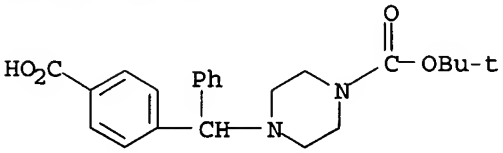
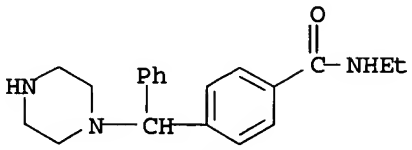
RX(26) OF 401



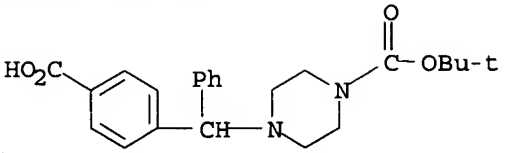
(step 1)

1. Et3N, ClCO2Bu-i, THF
2. EtNH2
3. F3CCO2H, CH2Cl2



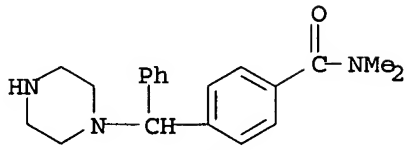
69%

RX(27) OF 401



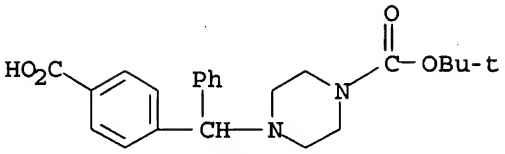
(step 1)

1. Et3N, ClCO2Bu-i, THF
2. Me2NH, THF
3. F3CCO2H, CH2Cl2



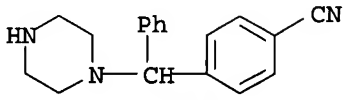
97%

RX(28) OF 401



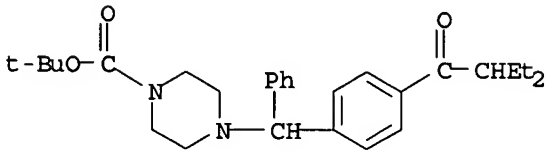
(step 1)

1. Et3N, ClCO2Bu-i, THF
2. NH3, CH2Cl2
3. Pyridine, (CF3CO)2O, THF
4. HCl, MeOH

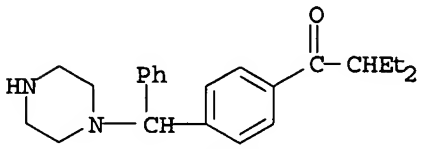


49%

RX(39) OF 401



HCl, AcOH, Water



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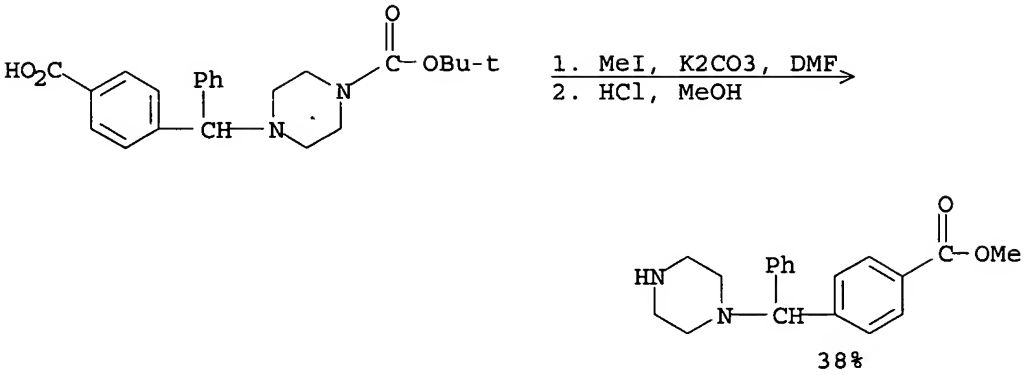
RX(148) OF 401 - 2 STEPS



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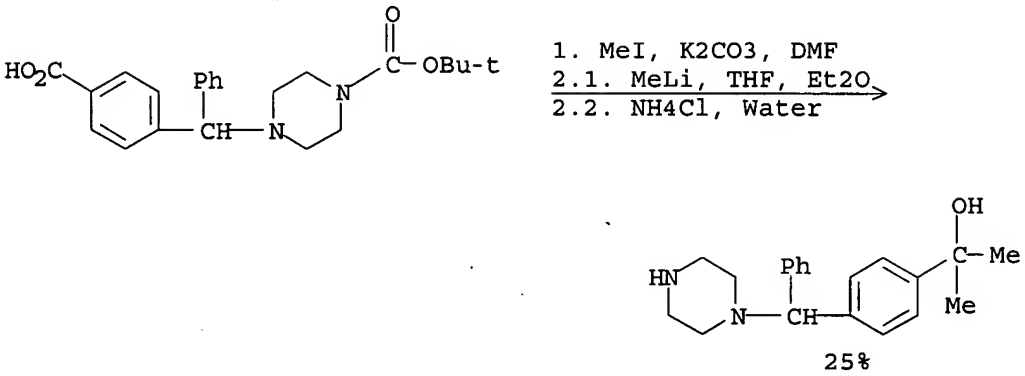
RX(149) OF 401 - 2 STEPS



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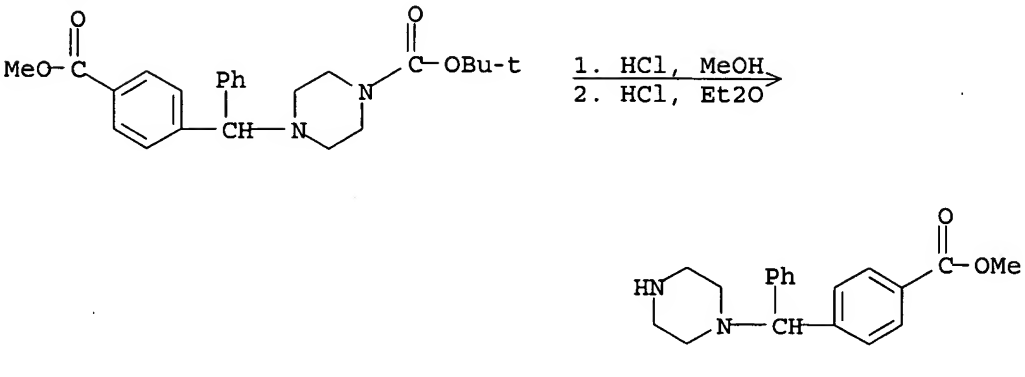
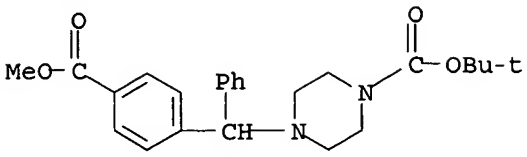
RX(150) OF 401 - 2 STEPS

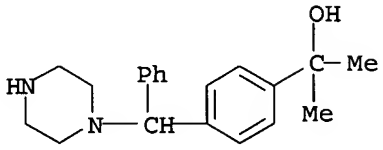


2 HCl

RX(151) OF 401 - 2 STEPS

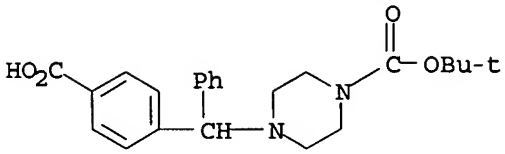


1.1. MeLi, THF, Et2O
1.2. NH4Cl, Water
2. HCl, Et2O

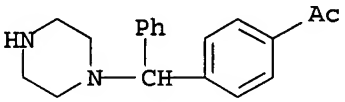


2 HCl

RX(152) OF 401 - 2 STEPS

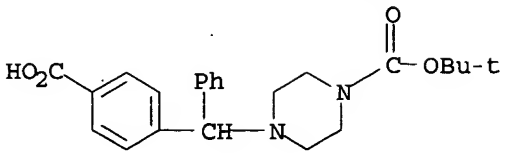


1.1. MeLi, THF, Et2O
1.2. Me3SiCl
1.3. NH4Cl, Water
2. HCl, Et2O

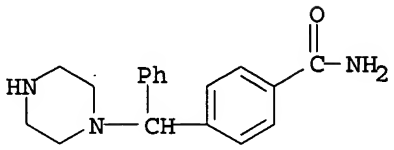


2 HCl

RX(153) OF 401 - 2 STEPS

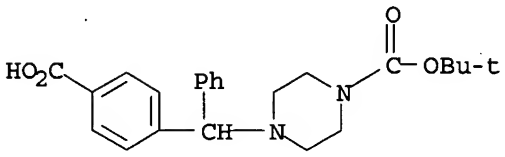


1.1. Et3N, ClCO2Bu-i, THF
1.2. NH3, CH2Cl2
1.3. F3CCO2H, CH2Cl2
2. HCl, Et2O

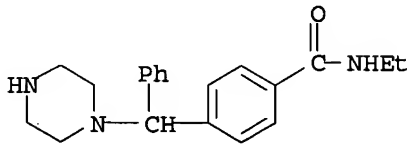


2 HCl

RX(154) OF 401 - 2 STEPS

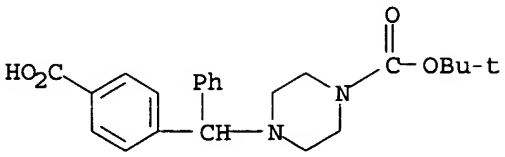


1.1. Et3N, ClCO2Bu-i, THF
1.2. EtNH2
1.3. F3CCO2H, CH2Cl2
2. HCl, Et2O

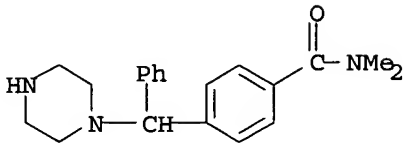


2 HCl

RX(155) OF 401 - 2 STEPS

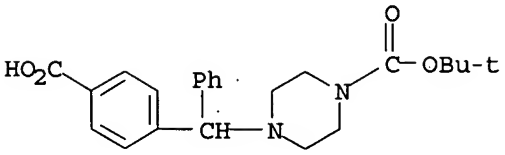


1.1. Et3N, ClCO2Bu-i, THF
1.2. Me2NH, THF
1.3. F3CCO2H, CH2Cl2
2. HCl, Et2O

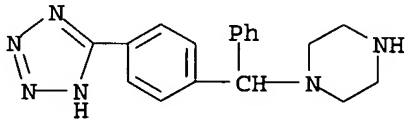


2 HCl

RX(156) OF 401 - 2 STEPS

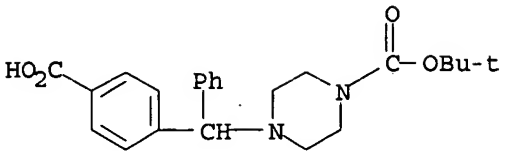


1.1. Et3N, ClCO2Bu-i, THF
1.2. NH3, CH2Cl2
1.3. Pyridine, (CF3CO)2O, THF
1.4. HCl, MeOH
2.1. R:1118-03-2, PhMe
2.2. R:1118-03-2
2.3. HCl, MeOH

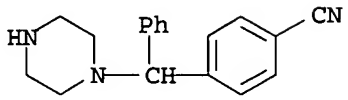


22%

RX(157) OF 401 - 2 STEPS

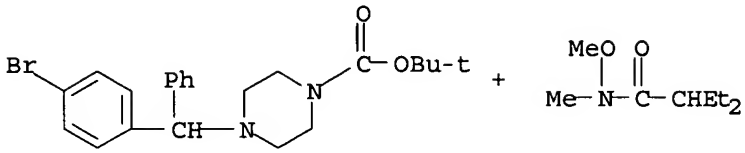


1.1. Et3N, ClCO2Bu-i, THF
1.2. NH3, CH2Cl2
1.3. Pyridine, (CF3CO)2O, THF
1.4. HCl, MeOH
2. HCl, Et2O, MeOH

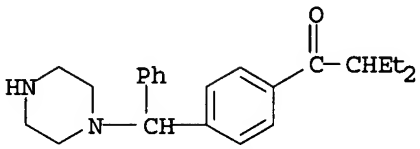


2 HCl

RX(166) OF 401 - 2 STEPS



1.1. BuLi, THF, Hexane
1.2. THF
1.3. NH4Cl, Water
2. HCl, AcOH, Water



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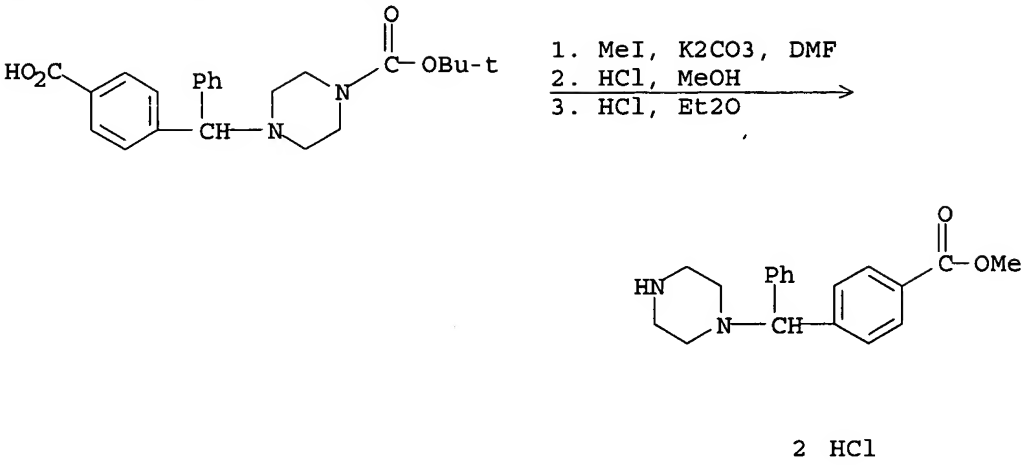
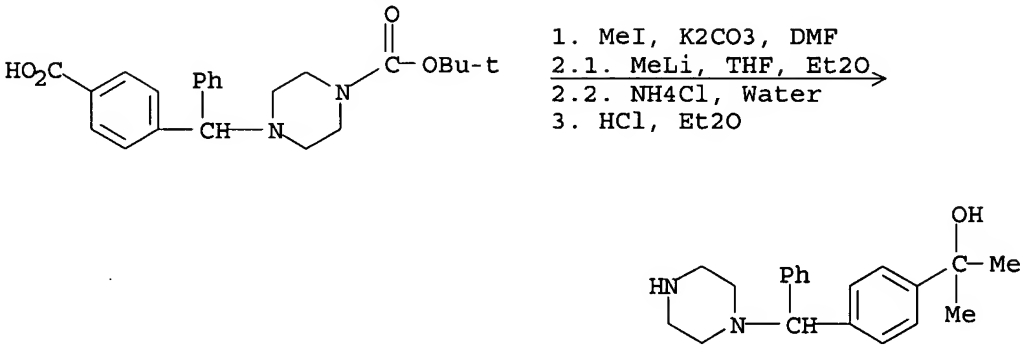
RX(294) OF 401 - 3 STEPS



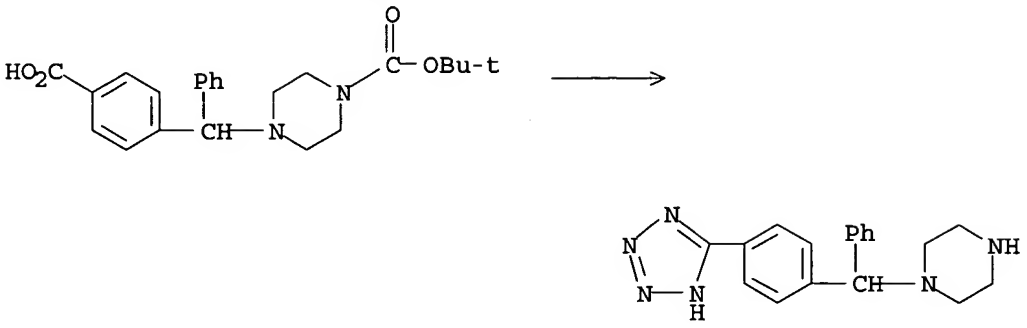
2 HCl

RX(295) OF 401 - 3 STEPS



2 HCl

RX(298) OF 401 - 3 STEPS



2 HCl

=> d 1-2 bib

L5 ANSWER 1 OF 2 CASREACT COPYRIGHT 2003 ACS
AN 138:4616 CASREACT
TI Preparation of 4-(phenyl-piperazinyl-methyl)-benzamides as .delta. opioid receptor agonists for the treatment of pain, anxiety or gastrointestinal disorders
IN Brown, William; Walpole, Christopher; Plobeck, Niklas
PA Astrazeneca Ab, Swed.
SO PCT Int. Appl., 40 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2002094794	A1	20021128	WO 2002-SE956	20020516

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRAI SE 2001-1772 20010518
SE 2001-3820 20011115
OS MARPAT 138:4616
RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 2 CASREACT COPYRIGHT 2003 ACS
AN 134:4912 CASREACT
TI New Diarylmethylpiperazines as Potent and Selective Nonpeptidic .delta. Opioid Receptor Agonists with Increased In Vitro Metabolic Stability
AU Plobeck, Niklas; Delorme, Daniel; Wei, Zhong-Yong; Yang, Hua; Zhou, Fei; Schwarz, Peter; Gawell, Lars; Gagnon, Helene; Pelcman, Benjamin; Schmidt, Ralf; Yue, Shi Yi; Walpole, Christopher; Brown, William; Zhou, Edward; Labarre, Maryse; Payza, Kemal; St-Onge, Stephane; Kamassah, Augustus; Morin, Pierre-Emmanuel; Projean, Denis; Ducharme, Julie; Roberts, Edward
CS Departments of Chemistry and Pharmacology, Astra Zeneca R&D Montreal, Saint-Laurent, QC, H4S 1Z9, Can.
SO Journal of Medicinal Chemistry (2000), 43(21), 3878-3894
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
RE.CNT 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/076448

=> log h

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	111.68	111.89

SESSION WILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 18:18:41 ON 17 JUL 2003